

Spin-polarized tunneling through a thin-film

Alireza Saffarzadeh*

Department of Physics, Shahid Beheshti University, 19839, Tehran, Iran
(12 June 2000)

The effect of spin-disorder scattering on perpendicular transport in a magnetic monolayer is considered within the single-site Coherent Potential Approximation (CPA). The exchange interaction between a conduction electron and localized moment of the magnetic ion is treated with the use of the s - f model. Electron-spin polarization is evaluated in the tunnel current which comes from the different densities of spin-up, spin-down conduction electrons at the Fermi level in a ferromagnetic semiconductor (EuS). Calculated results are compared with some tunneling experiments.

Keywords: Electron-spin polarization; Spin-filter effect; Spin-disorder scattering

I. INTRODUCTION

There has been renewed interest in spin-polarized transport over the last decade. This interest comes in part because of a wide range of novel phenomena, e.g., the giant and colossal magnetoresistance [1], spin-polarized tunneling experiments [2], and exchange coupling (or spin currents) [3]. One of the most fundamental properties of spin-polarized transport in a ferromagnet is the polarization in the density of states at the Fermi energy. This polarization enters either directly or indirectly into most transport calculations. In particular, since tunneling experiments measure the density of states, they should provide a direct measure of this polarization. In the case of ferromagnet-insulator-ferromagnet tunneling experiments one measures the product of the spin polarizations. However, in ferromagnet-insulator-superconductor tunneling experiments where the density of states in the superconductor is Zeeman split by a field in the plane of the film, one can in principle measure directly the spin polarization in the density of states. In these experiments the spin polarization was attributed to the difference in the spin densities of states of the itinerant electrons in the ferromagnets at the Fermi energy. In contrast to these experiments there have been a series of experiments where electron-spin polarization (ESP) of the tunneling current has been investigated between nonferromagnetic electrodes.

Ferromagnetic semiconductors, in particular the Eu chalcogenides, have been of great inter-

est because of their magnetic, optical, and transport properties [4,5]. Tunneling experiments using these materials as barriers demonstrated the spin polarization in the tunnel current by observing the decrease of junction resistance below the Curie temperature (T_c) of the barriers. Esaki *et al.* [6] studied the internal field-emission on metal-EuS-metal junctions at temperatures above and below EuS Curie temperature which is at 16.5 K for pure annealed thin films. They observed an increase of field-emission current as the temperature was lowered to below the magnetic ordering temperature of the barrier and interpreted it as caused by the decrease of barrier height when spin ordering takes place. Field-emission studies [7–10] on EuS-coated tungsten tips showed a high degree of polarization of the field-emitted electrons below the Curie temperature of EuS. In these experiments when EuS is used as a tunnel barrier, the conduction band splits into spin-up and spin-down subbands and the barrier height for these two subbands is changed. Since the tunneling process depends sensitively on the barrier height, the splitting of the EuS conduction band greatly increases the probability of tunneling for spin-up electrons and reduces that for spin-down electrons. This is called the “spin-filter” effect [11]. In favorable cases [12] the spin polarization in tunneling has exceeded 99%.

Electron-Spin Polarization, was studied theoretically by Takahashi [13]. Using the CPA for the s - f model he presented the dependence of the ESP on the magnetic field, the temperature, and the energy in the parabolic band model. Recently Metzke and Nolting [14] presented a new interpretation of the spin-filter effect using many-body theory on the s - f model in the film geometry, including an strong external electric field.

The purpose of the present paper is to develop a better theoretical framework for spin-polarized tunneling based on the coherent potential theory for the s - f model in the single band tight-binding model. Using this formalism we investigate density of states and tunneling spin-polarized through a EuS monolayer and the numerical calculated results are compared with the results of some experiments.

II. MODEL AND FORMALISM

We consider a system consisting of a ferromagnetic semiconductor (EuS) thin layer sandwiched between two semi-infinite lead wires.

*E-mail: a-saffarzadeh@cc.sbu.ac.ir

Both the thin layer and lead wires are described by a single-orbital tight-binding model with nearest neighbor hopping t on a simple cubic lattice with lattice constant a . We choose the (001) axis of the simple cubic structure to be normal to the layer and this direction is called z -direction hereafter.

We use the s - f (or s - d) model as it is believed to yield a good description for magnetic semiconductors. In this model the following Hamiltonian is used to describe the present system:

$$H = H_s + H_{sf} + H_f, \quad (1)$$

$$H_s = -t \sum_{\mathbf{r}n, \mathbf{r}'n', \sigma} c_{\mathbf{r},n,\sigma}^\dagger c_{\mathbf{r}',n',\sigma}, \quad (2)$$

$$H_{sf} = -I \sum_{\mathbf{r}, \sigma, \sigma'} (\sigma \cdot \mathbf{S}_{\mathbf{r},0})_{\sigma\sigma'} c_{\mathbf{r},0,\sigma}^\dagger c_{\mathbf{r},0,\sigma'}, \quad (3)$$

$$H_f = - \sum_{\mathbf{r}, \mathbf{r}'} J_{\mathbf{r}0, \mathbf{r}'0} \mathbf{S}_{\mathbf{r},0} \cdot \mathbf{S}_{\mathbf{r}',0} - g\mu_B H_0 \sum_{\mathbf{r}} S_{\mathbf{r},0}^z, \quad (4)$$

where \mathbf{r} and n denote the position in x - y plane and the layer index in the z -direction, respectively. Here H_s is the transfer energy of an s -electron between nearest-neighbor sites, $c_{\mathbf{r},n,\sigma}^\dagger$ ($c_{\mathbf{r},n,\sigma}$) is a creation (an annihilation) operator of an s -electron with spin $\sigma (= \uparrow, \downarrow)$ at site (\mathbf{r}, n) ; H_{sf} is the s - f exchange interaction between the s -electron and the f -spin where σ is a conduction electron spin operator, and I is the s - f exchange interaction energy. Each lattice point of the film is occupied by a localized magnetic moment, represented by a spin operator $\mathbf{S}_{\mathbf{r},0}$. The first term in (4) describes the direct exchange coupling of the Heisenberg type between these localized moments where $J_{\mathbf{r}0, \mathbf{r}'0}$ is an exchange integral; and the second term is the Zeeman energy when a magnetic field is applied in the z -direction. g is the Landé factor and μ_B is a Bohr magneton. The Zeeman effect on s -electrons are completely ignored. In this study H_f is treated in the molecular field approximation to obtain the magnetization at each temperature, ignoring the f -spin correlation. Thus we can define a normalized magnetic field in terms of the applied magnetic field by

$$h = \frac{(S+1)g\mu_B H_0}{3k_B T_c}. \quad (5)$$

We must note that $h=0.06$ corresponds to the magnetic field of 5 kOe.

The investigation of the spin-disorder scattering on the conduction electron in the bulk europium chalcogenides within the single-site CPA is not new, and was first performed by Nolting

[15]. In this approximation in order to treat electron scattering by thermally fluctuating localized spin at the layer, we consider a single f -spin located at site \mathbf{r} in an effective layered medium described by an effective potential (or coherent potential) which is site diagonal and takes the value Σ_\uparrow or Σ_\downarrow , according to the spin orientation of the s -electron. As in [16], we apply the condition that the average scattering of the s -electron by thermally fluctuating f -spin in the medium is zero. Thus we define the t -matrix of the s - f exchange interaction as

$$t_{\mathbf{r}} = v_{\mathbf{r}}(1 - \bar{G}v_{\mathbf{r}})^{-1}, \quad (6)$$

where \bar{G} is the effective Green's function of the layer in question. Here $t_{\mathbf{r}}$ is the complete scattering associated with the isolated potential $v_{\mathbf{r}}$ in the effective medium which is expressed as

$$v_{\mathbf{r}} = \sum_{\sigma\sigma'} [-I(\sigma \cdot \mathbf{S}_{\mathbf{r}})_{\sigma\sigma'} - \Sigma_\sigma \delta_{\sigma\sigma'}] c_{\mathbf{r},0,\sigma}^\dagger c_{\mathbf{r},0,\sigma'}. \quad (7)$$

We assume that the system is large enough and has translational invariance along x , y directions. We impose periodic boundary conditions along these directions and use the $|\mathbf{k}_\parallel, n\rangle$ representation, where $\mathbf{k}_\parallel = (k_x, k_y)$ is x - y components of the electron wave vector. In this representation the effective Green's function is \mathbf{k} -diagonal and can be given by [17]

$$\begin{aligned} F_\sigma(Z_+) &= \frac{1}{N_\parallel} \sum_{\mathbf{k}_\parallel} \langle \mathbf{k}_\parallel, 0, \sigma | \bar{G} | \mathbf{k}_\parallel, 0, \sigma \rangle \\ &= \frac{1}{N_\parallel} \sum_{\mathbf{k}_\parallel} \frac{1}{[G_{\mathbf{k}_\parallel}^{+(0)}]^{-1} - \Sigma_\sigma}, \end{aligned} \quad (8)$$

where N_\parallel is the number of sites in the plane of the layer, $Z_\pm = E \pm i\delta$ and $G_{\mathbf{k}_\parallel}^{+(0)}$ is the unperturbed Green's function propagating from left ($n < 0$) to right ($n > 0$) and is expressed as [18,19]

$$G_{\mathbf{k}_\parallel}^{+(0)} = \frac{1}{i(2ta)\sin k_\perp a}, \quad (9)$$

where

$$-2t\cos k_\perp a = E + 2t(\cos k_x a + \cos k_y a). \quad (10)$$

Here, δ is a small positive number and the summation includes both propagating and evanescent states.

Using the elements of the t -matrix of the s - f exchange interaction, the coherent potential, Σ_σ , in the thin layer (at $n=0$) can be determined by the following equations [16]:

$$\langle \langle \mathbf{k}_\parallel, 0, \uparrow | t_{\mathbf{r}} | \mathbf{k}_\parallel, 0, \uparrow \rangle \rangle_T = 0, \quad (11)$$

$$\left\langle \langle \mathbf{k}_{\parallel}, 0, \downarrow | t_{\mathbf{r}} | \mathbf{k}_{\parallel}, 0, \downarrow \rangle \right\rangle_T = 0, \quad (12)$$

where the bracket $\langle \dots \rangle_T$ means the thermal average. These equations can be transformed into the equations to determine Σ_{\uparrow} and Σ_{\downarrow} [16]. Once Σ_{σ} is determined, F_{σ} is obtained using Eq. (8). In the single-site approximation, the tunneling density of states for spin σ electron is calculated by

$$D_{\sigma}(E) = -\frac{1}{\pi} \text{Im} F_{\sigma}(E + i\delta), \quad (13)$$

and should satisfy the following equation in all of the present numerical calculations

$$\int_{-\infty}^{+\infty} D_{\sigma}(E) dE = 1.0. \quad (14)$$

We must note that in this work the spin flip of the s -electron is taken into account in the t -matrix formula, but the spin flip of the f -spin is neglected because the f -spin is treated as a classical spin.

We are now at the position to calculate the actual spin polarization for a ferromagnetic semiconductor as a function of temperature. An ensemble of electrons is said to have electron spin polarization when they show a preferential spin direction. ESP is described by the vector \mathbf{P} in the preferential direction, whose magnitude is given by

$$P = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}}, \quad (15)$$

where $N_{\uparrow}(N_{\downarrow})$ is the number of emitted electrons with spin-up (down). This quantity is obtained in experiments when the conduction band of EuS is almost empty. Then it is reasonable to assume that $N_{\uparrow}/N_{\downarrow}$ is equal to $D_{\uparrow}(E_F)/D_{\downarrow}(E_F)$, where $D_{\sigma}(E_F)$ is the density of states at the Fermi energy. Using these definitions, the polarization of the tunneling density of states is given by

$$P = \frac{D_{\uparrow}(E_F) - D_{\downarrow}(E_F)}{D_{\uparrow}(E_F) + D_{\downarrow}(E_F)}. \quad (16)$$

In this investigation E_F corresponds to the energy equivalent to almost the bottom of the conduction band.

III. NUMERICAL RESULTS

In numerical calculations we adopted the following values for EuS: $a = 5.97$ Å, $T_c = 16.5$ K [9], $S = 7/2$, $I = 0.1$ eV, $W = 0.9$ eV [20]. Here W is bandwidth and is $12t$. Note that following Refs. [17] and [18], the energy is measured in

units of ta . The small imaginary part of the energy is chosen $\delta = 0.02$ to simplify the numerical calculations.

In Fig. 1, the results of the density of states calculated in the present study is depicted as a function of the energy for $T = 0, 0.85 T_c$ and T_c Fig. 1(a)-(c) with no external magnetic field and at $T = 1.2 T_c$ Fig. 1(d) with a magnetic field of 5 kOe. According to the first order perturbation theory of the EuS conduction band, the ideal spin polarization of 100% for all temperatures below T_c and 0% above is expected where the band splits into two completely spin-polarized subbands. Present results show that at $T \geq T_c$ when magnetic field is zero, magnetization is zero and there is not any spin splitting between the two subbands. As the magnetization increases from paramagnetic state, the density of states for up-spin band shifts upward and for down-spin band shifts downward. The reason is that by decreasing the temperature the number of up-spin electrons participate in tunneling procedure increase but for down-spin it decreases.

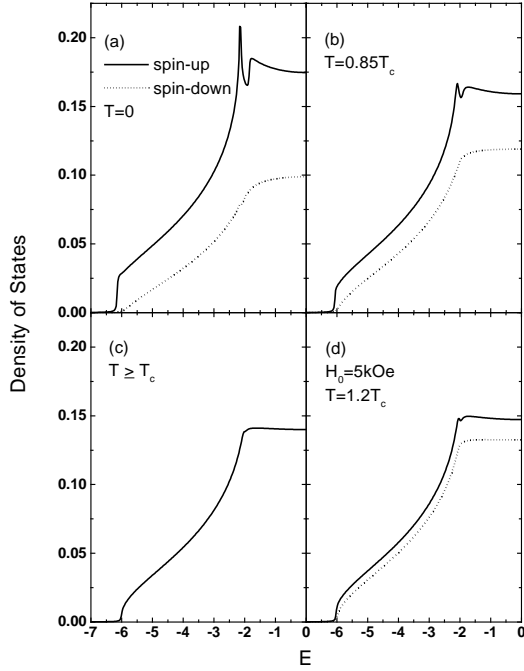


FIG. 1. The density of states as a function of energy without (curve a–c) and with the applied magnetic field (curve d) at the various temperatures. Here only the results for $E_F \leq 0$ are shown since the results for $E_F \geq 0$ are symmetric about the band center $E_F = 0$.

These curves show that a spin gap does not exist for both the conduction electron directions, i.e., even at zero temperature the spin-down

band has a tail extending down to the spin-up band edge as is already evidenced in CPA results of Nolting [15] in bulk europium chalcogenides. Consequently the relative conduction electron spin polarization does not reach the ideal value of 100%. The existence of the band tail suggests the spin-flip scattering to play an important role in the spin-polarized transport. The oscillations at the density of states are the effects of the van Hove singularities which appear at $E=\pm 2.0$.

In this investigation the spin flip of the f -spin was ignored since the f -spin was treated as a classical spin. Thus the present study cannot recover the existence of a spin polaron peak in the density of states as Metzke and Nolting [14] reported.

When the temperature is far below T_c , the spin filter effect in EuS polarizes the tunnel current even when no magnetic field is applied. The effect of the external magnetic field is only to remove the domain structure. In Fig. 2(a) and (b), we show the results for tunneling spin polarized for $E_F=-6.07$ as a function of temperature together with the field-ESP experiment data for EuS at $H_0=0$ [8,9] and $H_0=5$ kOe [10] respectively. The agreement between the calculated results and experiment data is satisfactory. The difference between experiment results and present theory at around T_c and at paramagnetic temperatures is due to ignoring the exchange scattering due to the correlation of f -spins and use of monolayer instead of multilayers. The inset of Fig. 2(b) shows the tunneling spin polarized as a function of s -electron energy at $T=0$. This result, together with the experiment data, strongly suggest that the ESP in field-emission studies corresponds to the P value for low electron energy ($E \leq -5.8$ in this study). For energy less than this value the ESP is as high as 90% even at zero magnetic field.

On the other hand, experimental results show that the degree of field-ESP observed is much higher than that of photoemission (photo-ESP) [4,5]. In photo-ESP the electrons from $4f^7$ states by absorbing a photon transfer to the conduction band. Thus, most photoemitted electrons have higher energy than the energy of the bottom of the conduction band and are related to a large density of states. Therefore, as Fig. 1 and the inset of Fig. 2(b) show the degree of polarization of high-energy electrons such as $-5.8 \leq E \leq -5.0$, in the present study, is rather low.

Consequently the difference between the results of photo-ESP and field-ESP is due to the difference in the energies of electrons in the emission processes, which is consistent with the work of Takahashi [13] in bulk europium chalcogenides. These results are confirmed by experimental results of Kisker *et al.* [10] in which they showed that the low energy electrons are highly polarized, whereas the polarization degree of high energy electrons is rather low.

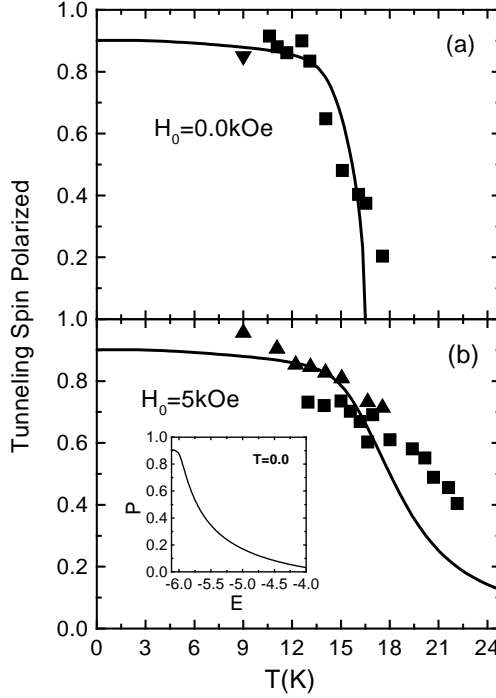


FIG. 2. The tunneling spin polarized as a function of temperature without (curve-a) and with the applied magnetic field (curve-b). The experimental results in curve-a (square and down-triangle symbols) are taken from Ref. 8 and Ref. 9 respectively and in curve-b (square and up-triangle) are taken from Ref. 10. The inset is a calculated result of the ESP as a function of energy.

IV. CONCLUDING REMARKS

In this study we attempted to explain the results of the tunneling spin polarized measurements based on the spin-polarized subbands picture for an EuS layer. Using the CPA for the s - f model we considered the effects of spin disorder on the perpendicular transport through a monolayer. Assuming a single band tight-binding model numerical calculations were performed for the density of states and tunneling spin polarized. The agreement between the calculated and some experiments results is satisfactory.

Throughout this investigation the effect of interface roughness that plays an important role in the giant magnetoresistance and the scattering due to the correlation of f -spins are not taken into account.

- [1] M. N. Baibich, J. M. Broto, A. Fert, Nguyen Van Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, *Phys. Rev. Lett.* **61** (1988) 2472.
- [2] M. Julliere, *Phys. Lett. A* **54** (1975) 225.
- [3] P. Grünberg, R. Schreiber, Y. Pang, M. B. Brodsky, and H. Sowers, *Phys. Rev. Lett.* **57** (1986) 2442.
- [4] P. Wachter, *Handbook on the Physics and Chemistry of Rare Earths*, edited by K. A. Gschneider, Jr. and L. Eyring, North-Holland, Amsterdam, 1979 (Chapter 19).
- [5] A. Mauger and C. Godart, *Phys. Rep.* **141** (1986) 51.
- [6] L. Esaki, P. J. Stiles, and S. von Molnar, *Phys. Rev. Lett.* **19** (1967) 852.
- [7] N. Müller, W. Eckstein, W. Heiland, and W. Zinn, *Phys. Rev. Lett.* **29** (1972) 1651.
- [8] E. Kisker, G. Baum, A. H. Mahan, W. Raith, and K. Schröder, *Phys. Rev. Lett.* **36** (1976) 982.
- [9] G. Baum, E. Kisker, A. H. Mahan, W. Raith, and B. Reihl, *Appl. Phys.* **14** (1977) 149.
- [10] E. Kisker, G. Baum, A. H. Mahan, W. Raith, and B. Reihl, *Phys. Rev. B* **18** (1978) 2256.
- [11] J. S. Moodera, X. Hao, G. A. Gibson, and R. Meservey, *Phys. Rev. Lett.* **61** (1988) 637; X. Hao, J. S. Moodera, and R. Meservey, *Phys. Rev. B* **42** (1990) 8235.
- [12] J. S. Moodera, R. Meservey, and X. Hao, *Phys. Rev. Lett.* **70** (1993) 853.
- [13] M. Takahashi, *Phys. Rev. B* **56** (1997) 7389.
- [14] R. Metzke and W. Nolting, *Phys. Rev. B* **58** (1998) 8579.
- [15] W. Nolting, *Phys. Status Solidi B* **96** (1979) 11.
- [16] M. Takahashi and K. Mitsui, *Phys. Rev. B* **54** (1996) 11298.
- [17] A. Brataas and G. E. W. Bauer, *Phys. Rev. B* **49** (1994) 14684.
- [18] D. S. Fisher and P. A. Lee, *Phys. Rev. B* **23** (1981) 6851.
- [19] H. Itoh, J. Inoue, Y. Asano, and S. Maekawa, *J. Magn. Magn. Mater.* **156** (1996) 343.
- [20] W. Nolting, U. Dubil, and M. Matlak, *J. Phys. C* **18** (1985) 3687.